wwPDB EM Validation Summary Report

Dec 10, 2022 – 10:53 am GMT

PDB ID	:	5G04
EMDB ID	:	EMD-3385
Title	:	Structure of the human APC-Cdc20-Hsl1 complex
Authors	:	Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on	:	2016-03-16
Resolution	:	4.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

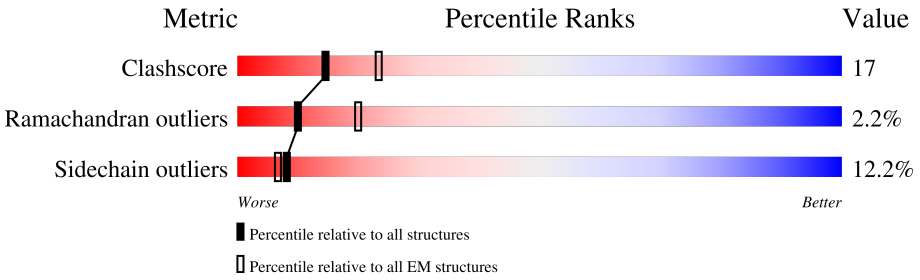
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1944	41% 26% 6% 26%
2	B	84	98% 69% 23% 6%
3	C	597	8% 44% 34% 10% 12%
3	P	597	5% 53% 24% 5% 18%
4	D	121	26% 17% 55%
5	E	110	35% 15% 49%
6	F	824	41% 17% 40%
6	H	824	41% 16% 41%

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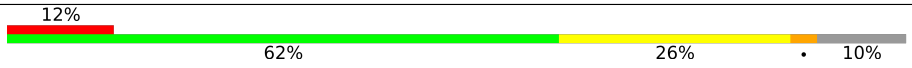
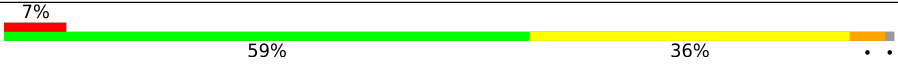
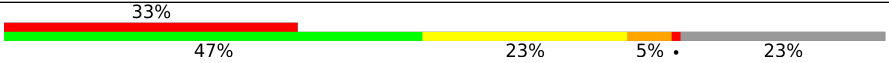
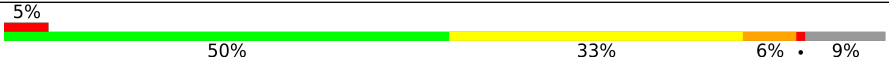
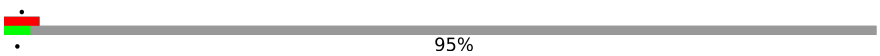
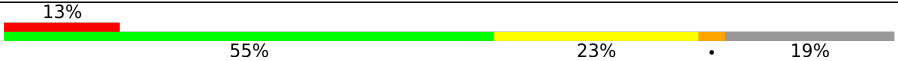
Mol	Chain	Length	Quality of chain
7	G	85	
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	184	
11	M	74	
12	N	822	
13	O	755	
14	R	499	
15	S	206	
16	X	599	
16	Y	599	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 65481 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1437	Total	C	N	O	S	0	0
			10925	7025	1849	1977	74		

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	1	0
			649	416	117	99	17		

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	524	Total	C	N	O	S	0	0
			4306	2774	727	781	24		
3	P	491	Total	C	N	O	S	0	0
			4039	2608	678	729	24		

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	55	Total	C	N	O	0	0
			436	277	73	86		

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			450	290	74	85	1		

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	498	Total	C	N	O	S	0	0
			3923	2514	664	719	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			213	133	40	39	1		
7	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	730	Total	C	N	O	S	0	0
			5709	3660	950	1066	33		

- Molecule 9 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2601	684	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2563	672	729	24		

- Molecule 10 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	182	Total	C	N	O	S	0	0
			1435	898	263	268	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	ARG	deletion	UNP Q9UM13

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	59	Total	C	N	O	S	0	0
			493	310	79	102	2		

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	631	Total	C	N	O	S	0	0
			4837	3067	880	868	22		

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	685	Total	C	N	O	S	0	0
			5395	3440	940	987	28		

- Molecule 14 is a protein called CELL DIVISION CYCLE PROTEIN 20 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	370	Total	C	N	O	S	2	0
			2869	1801	524	532	12		

- Molecule 15 is a protein called PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	S	10	Total	C	N	O	0	0
			72	42	14	16		

- Molecule 16 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	484	Total	C	N	O	S	0	0
			3767	2390	649	704	24		
16	Y	496	Total	C	N	O	S	0	0
			3859	2444	666	724	25		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

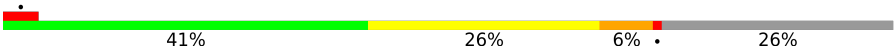
Mol	Chain	Residues	Atoms		AltConf
17	B	3	Total	Zn	0
			3	3	

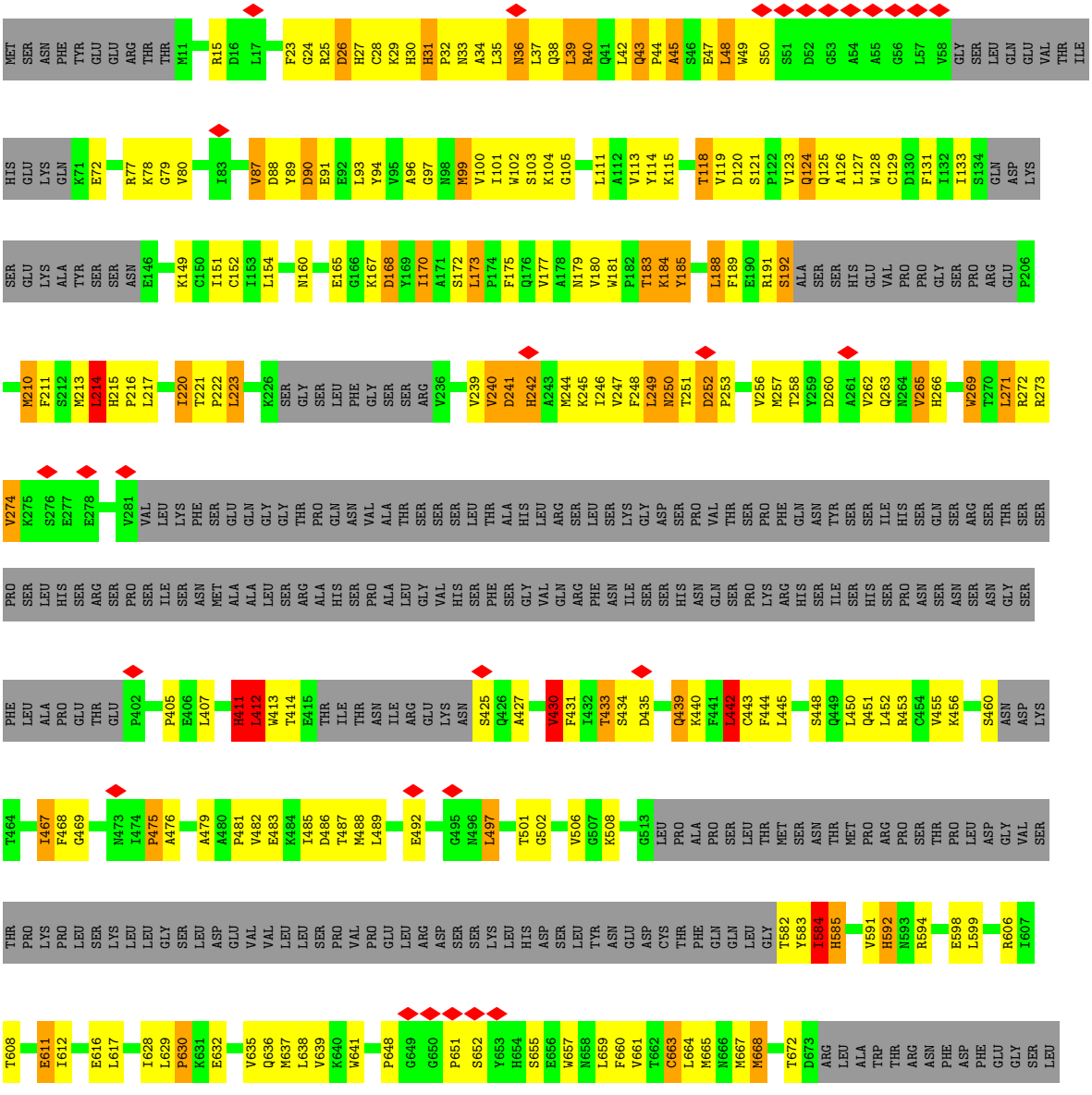
3 Residue-property plots (i)

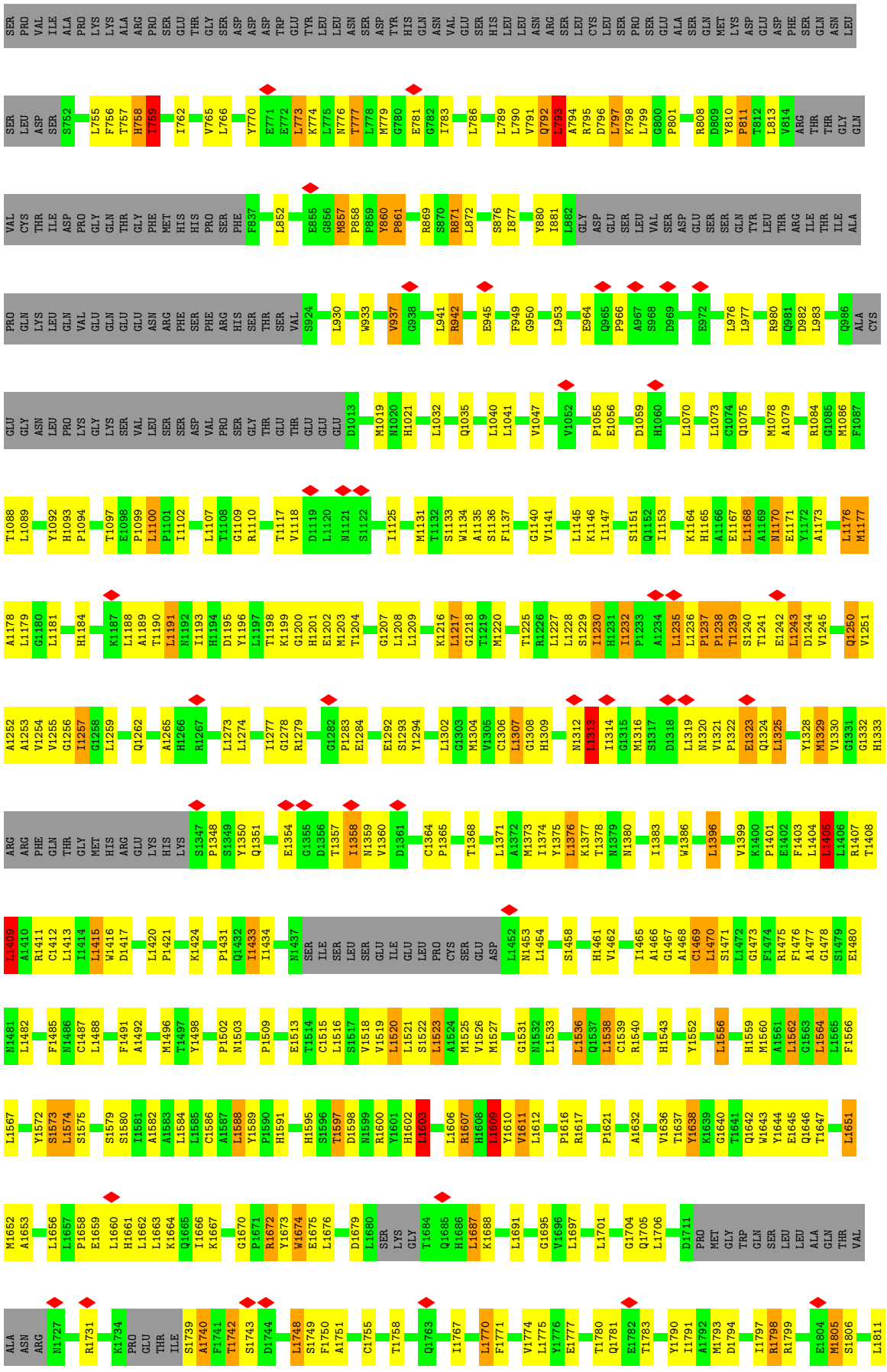
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

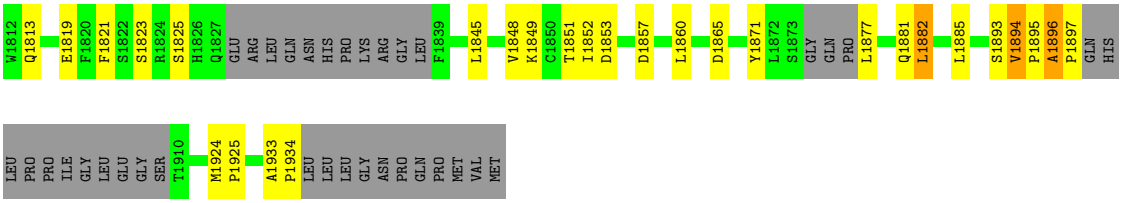
• Molecule 1: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1

Chain A:



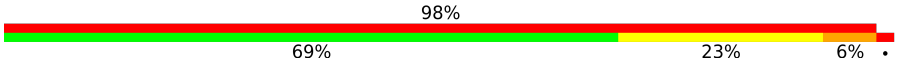


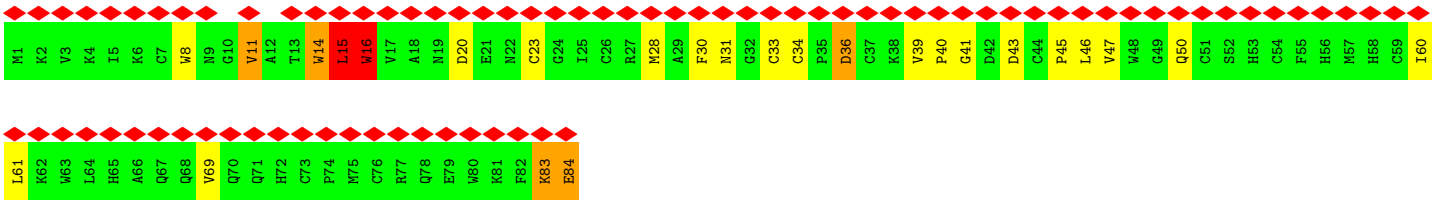




• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

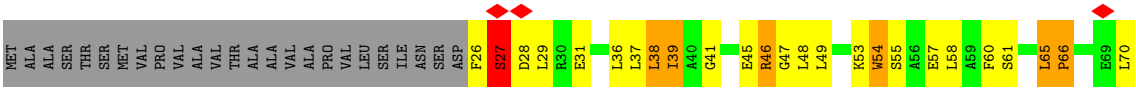
Chain B:

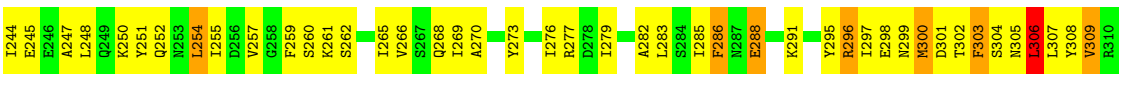


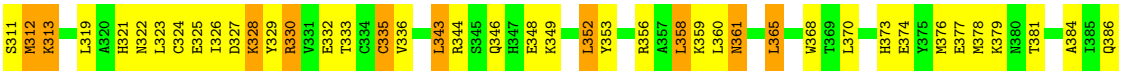


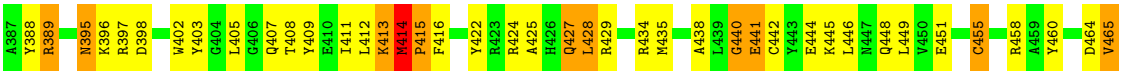
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

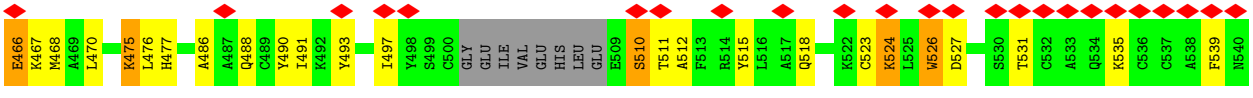
Chain C:

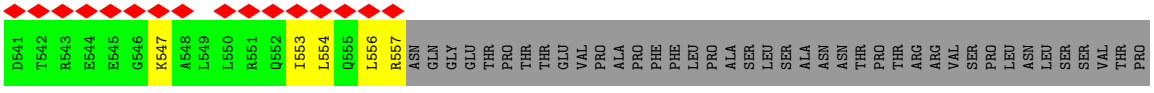






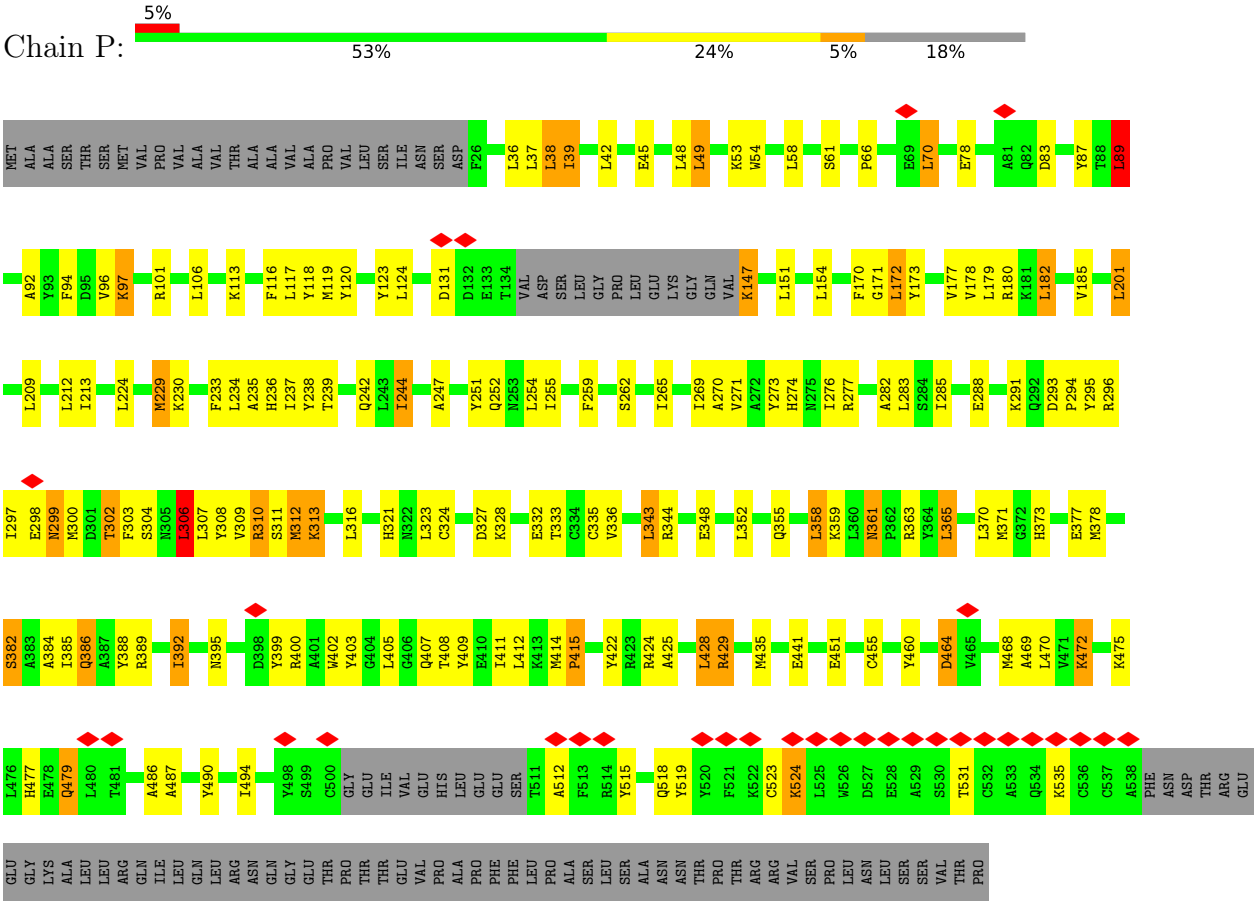






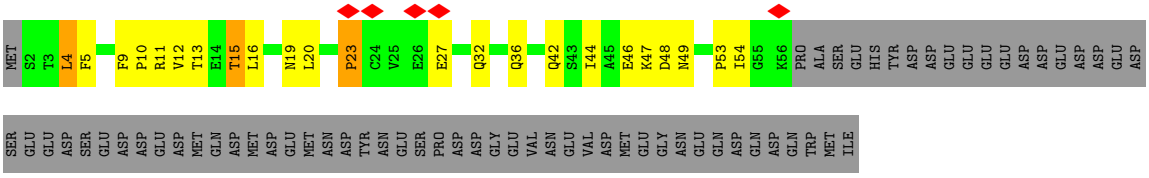
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain P:



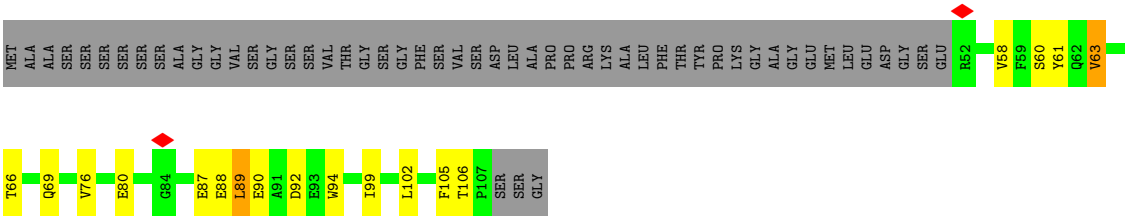
• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D:



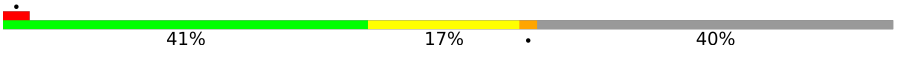
• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

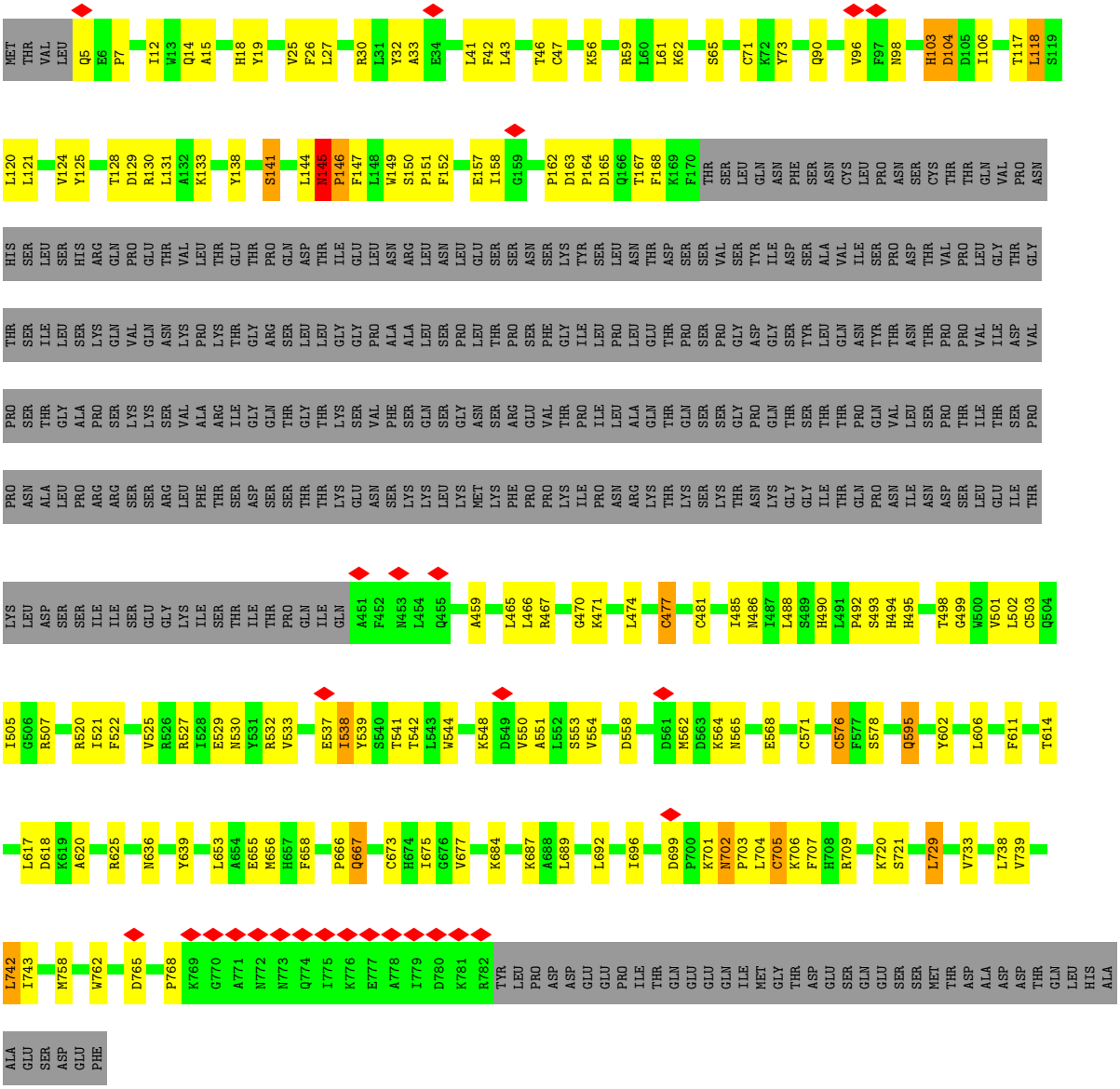
Chain E:



• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

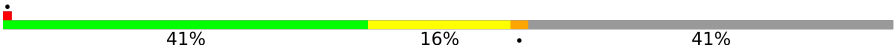
Chain F:

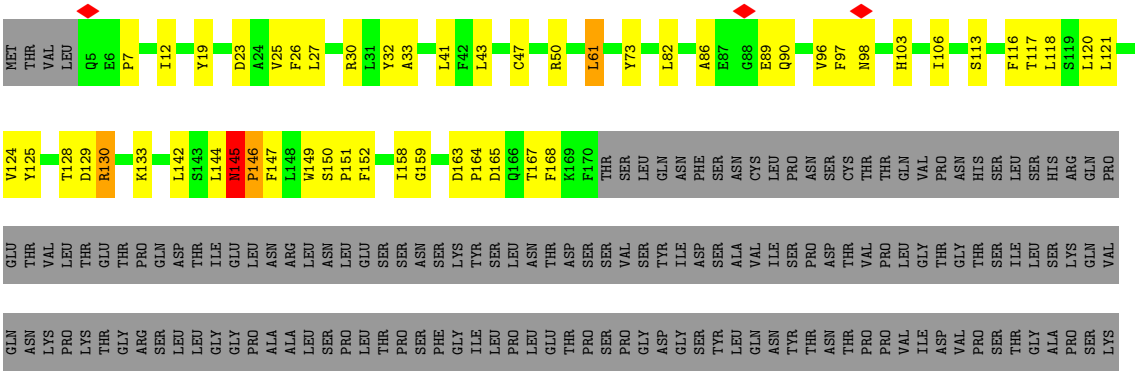


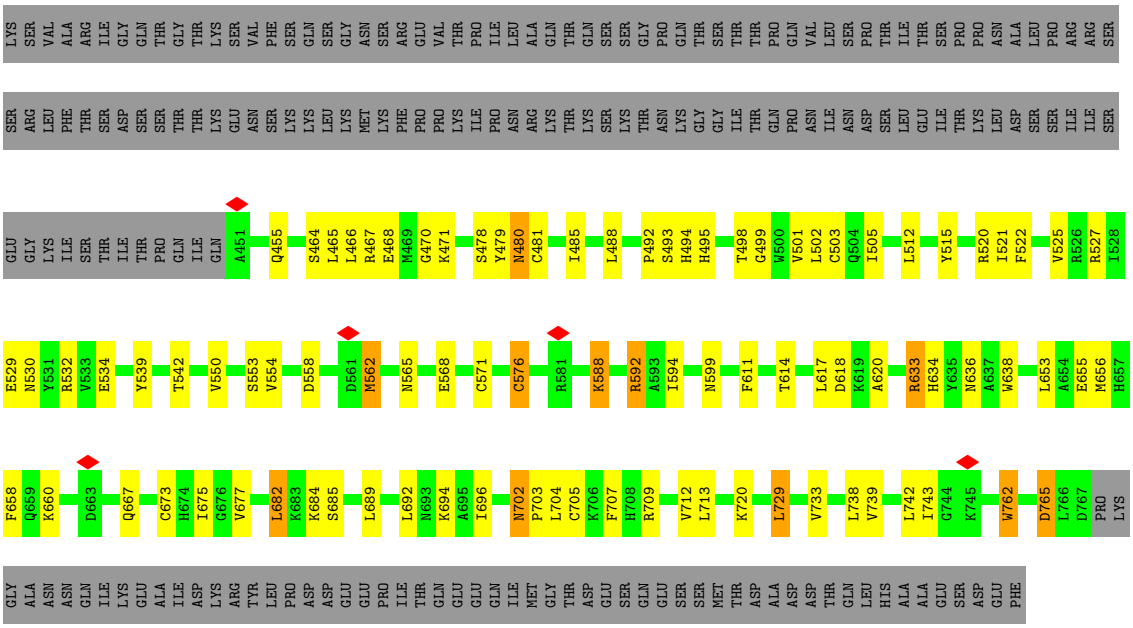


• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain H:

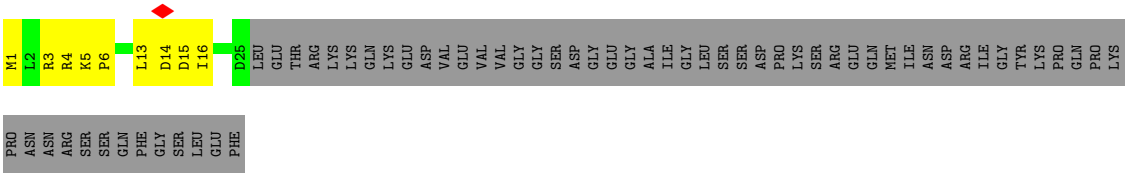






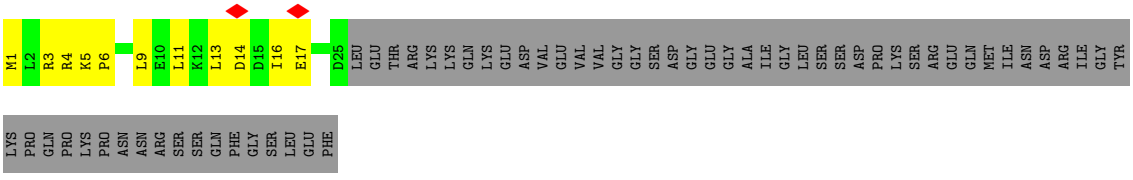
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G:



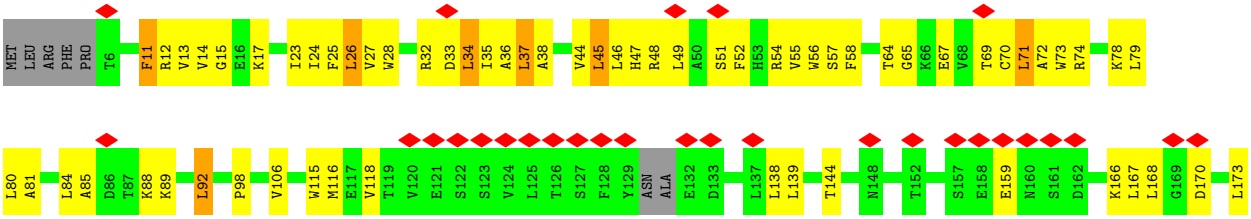
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

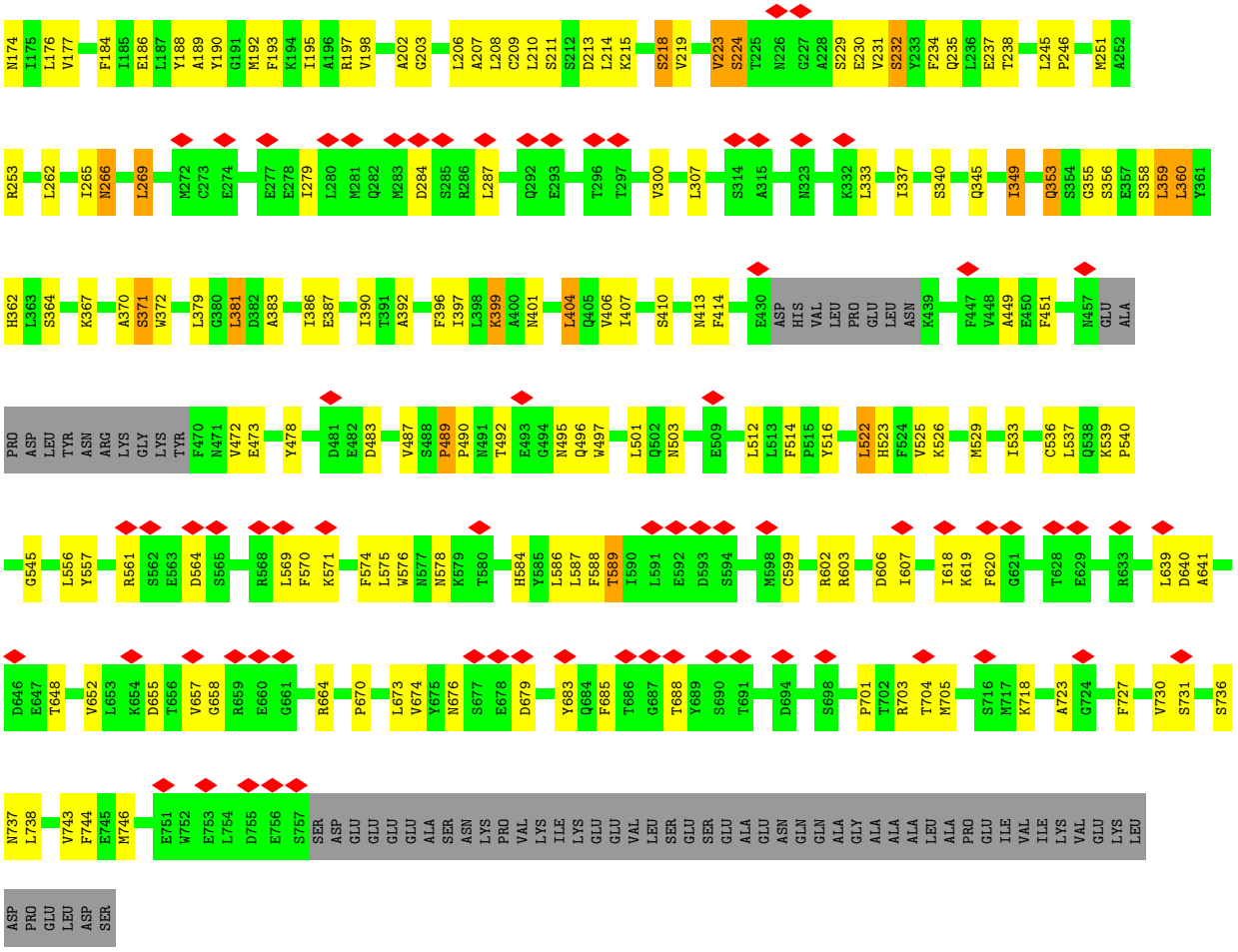
Chain W:



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

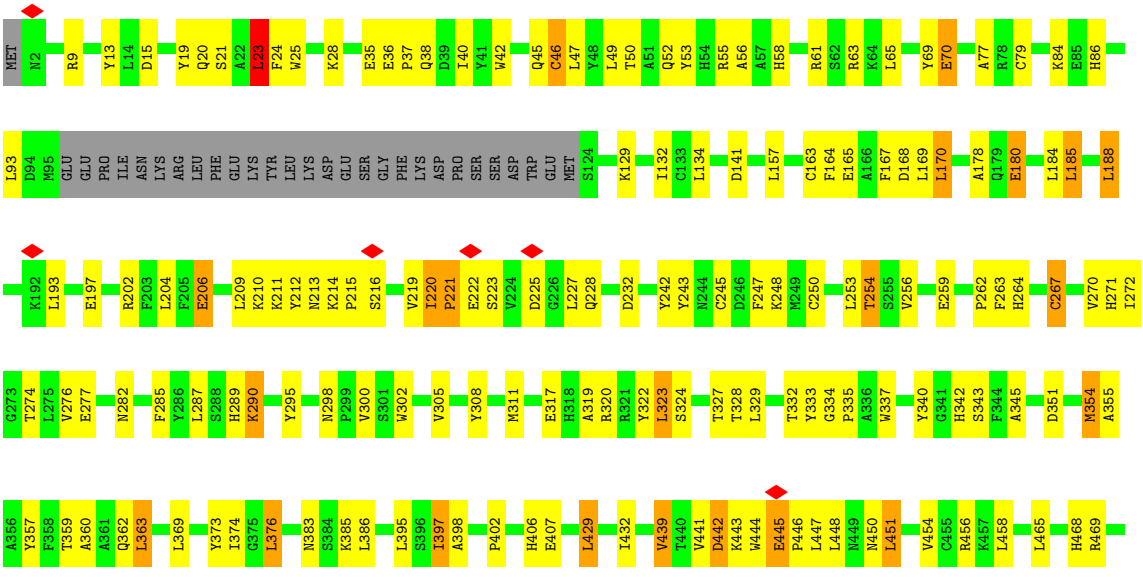
Chain I:

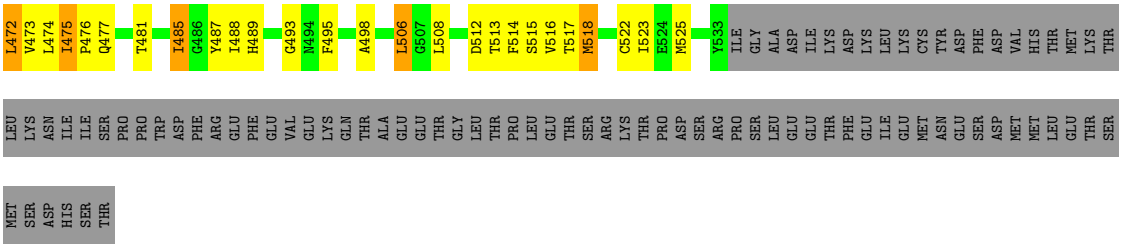




• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

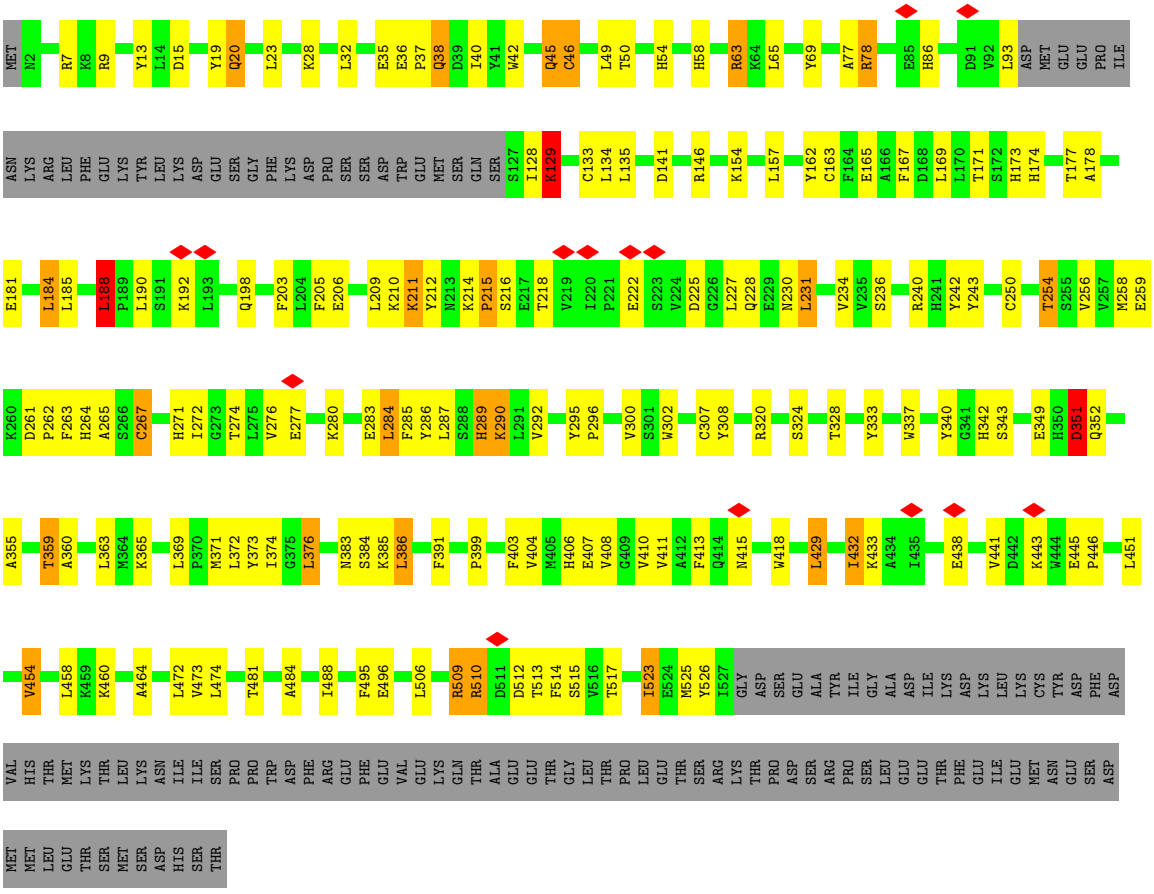
Chain J:





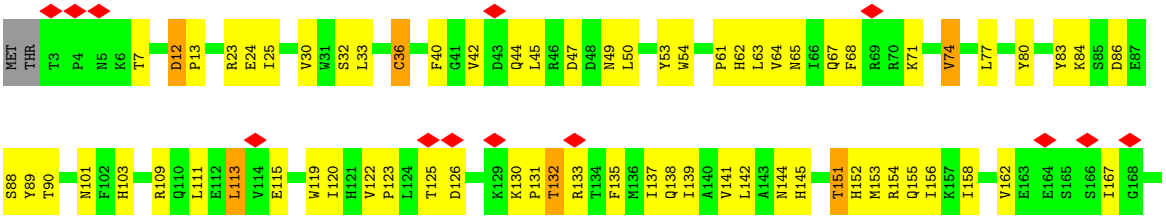
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

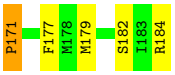
Chain K:



• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

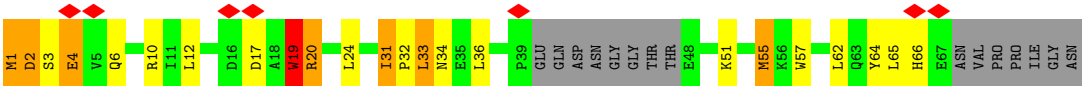
Chain L:





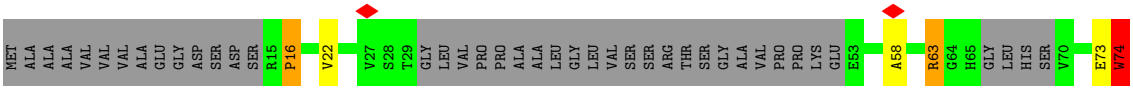
• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

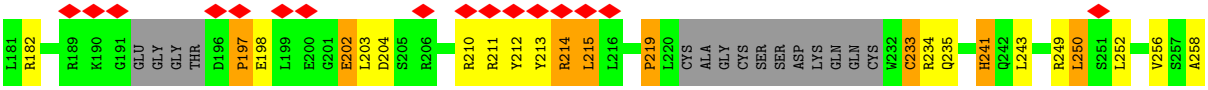
Chain M:

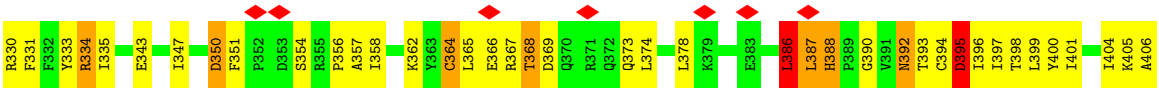


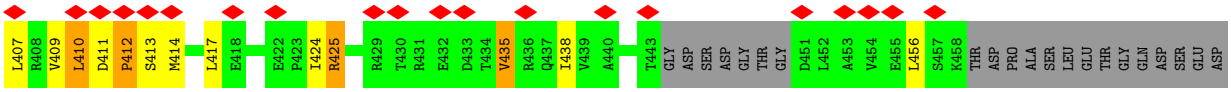
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

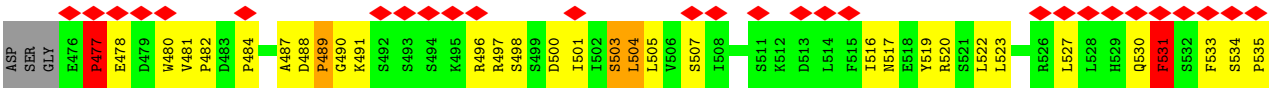
Chain N:

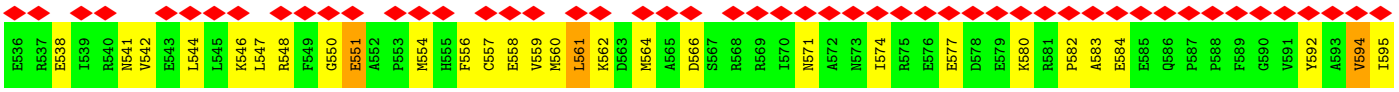


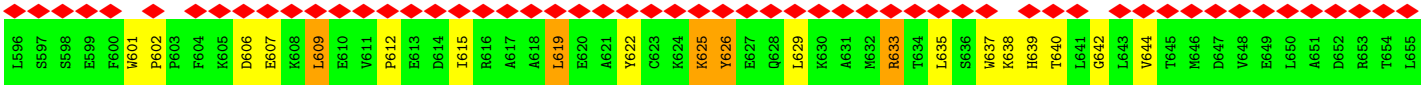


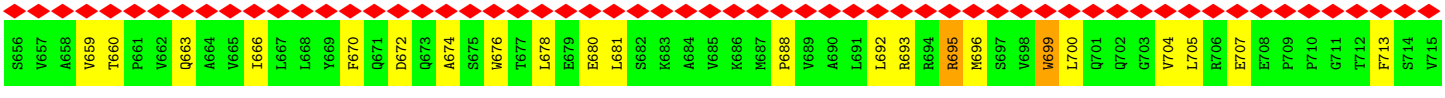


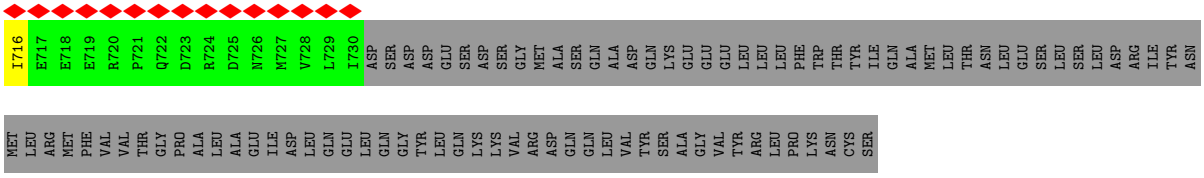






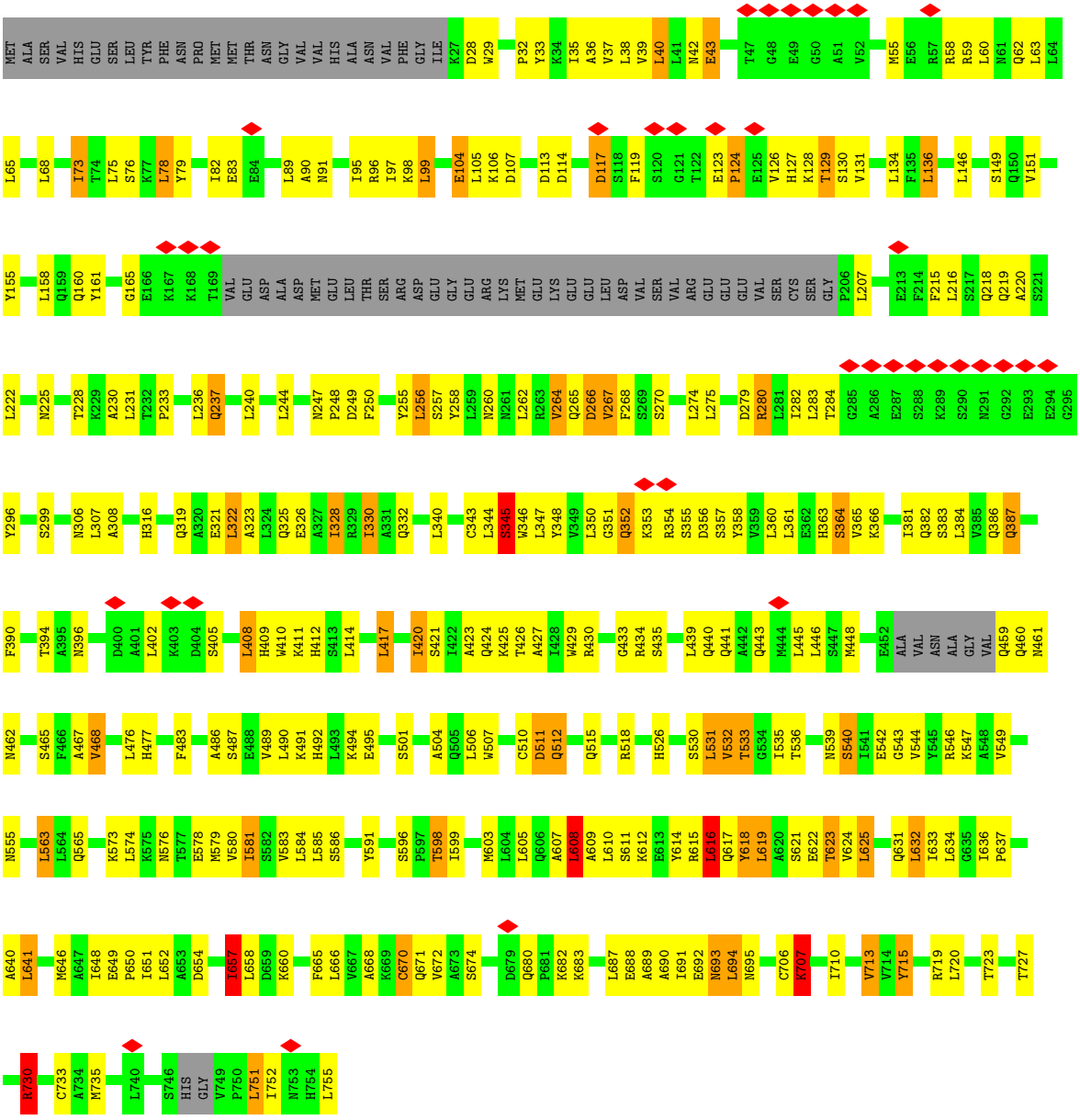






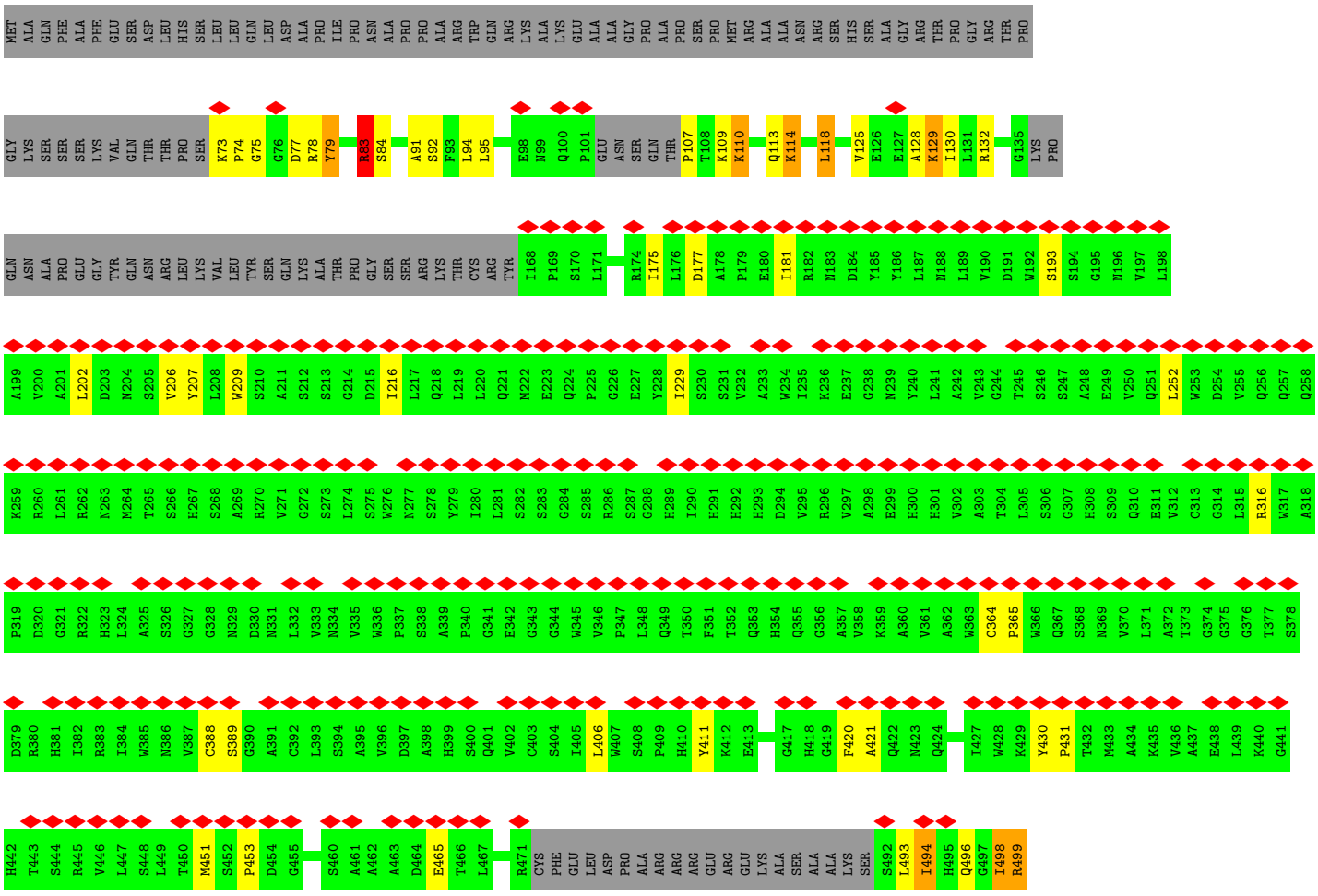
• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O:

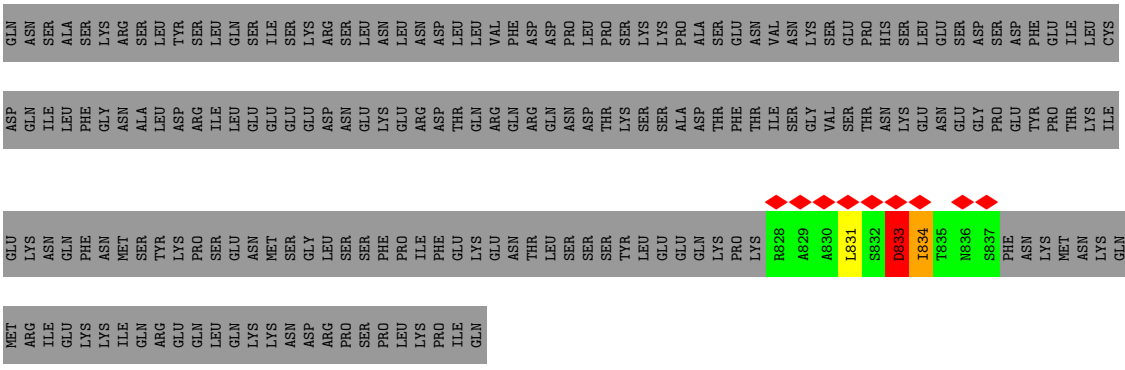


• Molecule 14: CELL DIVISION CYCLE PROTEIN 20 HOMOLOG

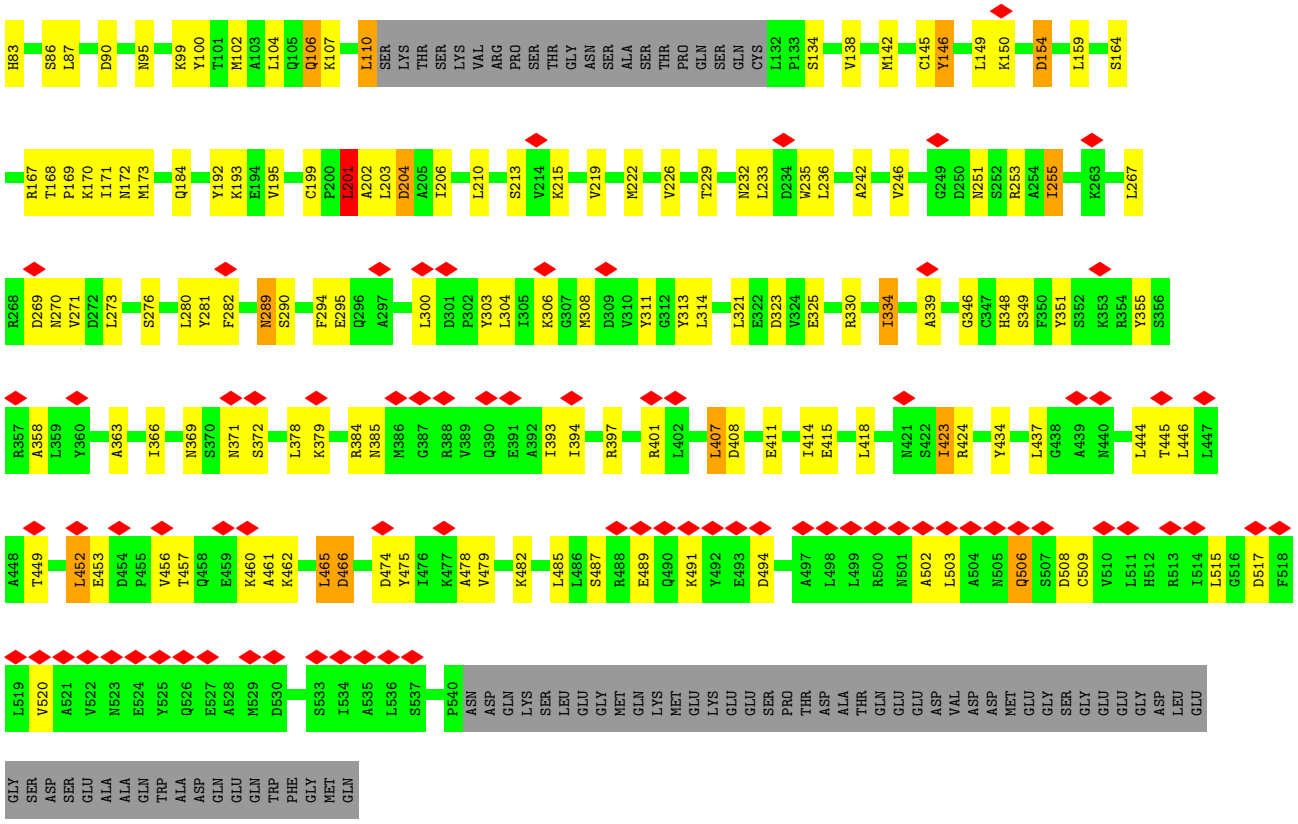
Chain R:



• Molecule 15: PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1

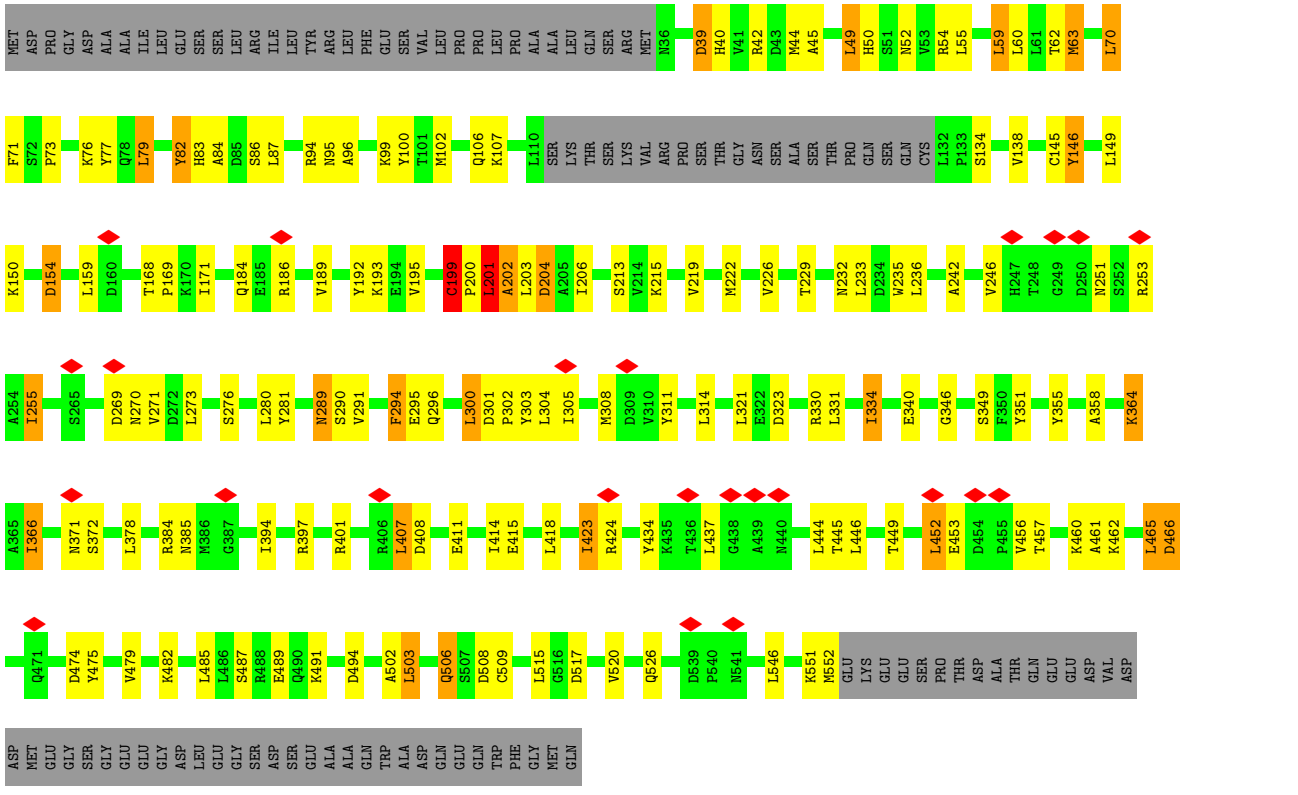


• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7



• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	179660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.392	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	386.24, 386.24, 386.24	wwPDB
Map dimensions	284, 284, 284	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	0/11165	0.89	29/15204 (0.2%)
2	B	0.67	0/674	0.91	0/913
3	C	0.65	0/4404	0.94	8/5945 (0.1%)
3	P	0.63	0/4134	0.91	7/5583 (0.1%)
4	D	0.58	0/446	0.85	1/610 (0.2%)
5	E	0.57	0/459	0.78	0/619
6	F	0.58	0/4013	0.83	4/5428 (0.1%)
6	H	0.59	0/3942	0.82	3/5326 (0.1%)
7	G	0.59	0/214	0.92	1/284 (0.4%)
7	W	0.64	0/214	0.86	0/284
8	I	0.65	0/5827	0.93	12/7899 (0.2%)
9	J	0.69	1/4146 (0.0%)	0.94	6/5616 (0.1%)
9	K	0.70	1/4086 (0.0%)	0.93	5/5534 (0.1%)
10	L	0.67	0/1468	0.88	1/1993 (0.1%)
11	M	0.63	1/502 (0.2%)	0.95	0/680
12	N	0.54	0/4915	0.88	15/6645 (0.2%)
13	O	0.61	1/5493 (0.0%)	0.92	14/7421 (0.2%)
14	R	0.54	2/2940 (0.1%)	0.72	1/3996 (0.0%)
15	S	0.50	0/71	1.09	1/95 (1.1%)
16	X	0.55	0/3826	0.80	6/5177 (0.1%)
16	Y	0.55	0/3919	0.82	10/5301 (0.2%)
All	All	0.61	6/66858 (0.0%)	0.88	124/90553 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	H	0	1
8	I	0	3
9	J	0	1
10	L	0	1
11	M	0	1
12	N	0	4
16	Y	0	1
All	All	0	15

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	268	PHE	CG-CD2	7.98	1.50	1.38
9	J	302	TRP	CB-CG	-6.32	1.38	1.50
14	R	79	TYR	CB-CG	5.73	1.60	1.51
11	M	19	TRP	CB-CG	5.53	1.60	1.50
14	R	79	TYR	CE1-CZ	5.37	1.45	1.38

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	358	LEU	CA-CB-CG	9.86	137.98	115.30
13	O	730	ARG	NE-CZ-NH1	9.15	124.88	120.30
3	C	440	GLY	N-CA-C	-8.87	90.94	113.10
9	K	351	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	1235	LEU	CA-CB-CG	8.41	134.65	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLN	Peptide
6	F	565	ASN	Peptide
6	H	565	ASN	Peptide
8	I	489	PRO	Peptide
8	I	658	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10925	0	10669	471	0
2	B	649	0	595	26	0
3	C	4306	0	4273	274	0
3	P	4039	0	3989	120	0
4	D	436	0	396	27	0
5	E	450	0	435	12	0
6	F	3923	0	3819	115	0
6	H	3853	0	3793	110	0
7	G	213	0	220	16	0
7	W	213	0	220	9	0
8	I	5709	0	5597	188	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	148	0
10	L	1435	0	1382	43	0
11	M	493	0	469	17	0
12	N	4837	0	4534	155	0
13	O	5395	0	5429	231	0
14	R	2869	0	2772	59	0
15	S	72	0	71	10	0
16	X	3767	0	3819	136	0
16	Y	3859	0	3908	150	0
17	B	3	0	0	0	0
All	All	65481	0	64247	2216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 2216 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:362:LYS:HG3	12:N:410:LEU:CD2	1.38	1.52
9:J:223:SER:CB	9:J:228:GLN:HE21	1.29	1.44
12:N:362:LYS:CG	12:N:410:LEU:HD23	1.60	1.31
12:N:362:LYS:CB	12:N:410:LEU:HD21	1.67	1.24
14:R:177:ASP:OD2	15:S:834:ILE:HD11	1.30	1.23

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1393/1944 (72%)	1186 (85%)	149 (11%)	58 (4%)	3 25
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2 23
3	C	520/597 (87%)	489 (94%)	23 (4%)	8 (2%)	10 45
3	P	485/597 (81%)	460 (95%)	20 (4%)	5 (1%)	15 53
4	D	53/121 (44%)	45 (85%)	7 (13%)	1 (2%)	8 40
5	E	54/110 (49%)	54 (100%)	0	0	100 100
6	F	494/824 (60%)	461 (93%)	25 (5%)	8 (2%)	9 44
6	H	477/824 (58%)	448 (94%)	22 (5%)	7 (2%)	10 45
7	G	23/85 (27%)	23 (100%)	0	0	100 100
7	W	23/85 (27%)	23 (100%)	0	0	100 100
8	I	722/808 (89%)	683 (95%)	34 (5%)	5 (1%)	22 61
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	19 58
9	K	489/620 (79%)	459 (94%)	24 (5%)	6 (1%)	13 49
10	L	180/184 (98%)	165 (92%)	11 (6%)	4 (2%)	6 37
11	M	55/74 (74%)	42 (76%)	10 (18%)	3 (6%)	2 21
12	N	601/822 (73%)	497 (83%)	58 (10%)	46 (8%)	1 14
13	O	677/755 (90%)	619 (91%)	46 (7%)	12 (2%)	8 41
14	R	361/499 (72%)	338 (94%)	20 (6%)	3 (1%)	19 58
15	S	8/206 (4%)	6 (75%)	0	2 (25%)	0 1
16	X	478/599 (80%)	463 (97%)	12 (2%)	3 (1%)	25 63
16	Y	492/599 (82%)	474 (96%)	14 (3%)	4 (1%)	19 58
All	All	8168/11057 (74%)	7474 (92%)	511 (6%)	183 (2%)	10 37

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ALA
1	A	241	ASP
1	A	274	VAL
1	A	411	HIS
1	A	413	TRP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1150/1720 (67%)	970 (84%)	180 (16%)	2 16
2	B	65/75 (87%)	54 (83%)	11 (17%)	2 14
3	C	452/520 (87%)	357 (79%)	95 (21%)	1 6
3	P	421/520 (81%)	363 (86%)	58 (14%)	3 20
4	D	46/115 (40%)	37 (80%)	9 (20%)	1 8
5	E	47/89 (53%)	37 (79%)	10 (21%)	1 6
6	F	407/727 (56%)	369 (91%)	38 (9%)	9 32
6	H	408/727 (56%)	374 (92%)	34 (8%)	11 38
7	G	23/77 (30%)	22 (96%)	1 (4%)	29 56
7	W	23/77 (30%)	22 (96%)	1 (4%)	29 56
8	I	620/730 (85%)	584 (94%)	36 (6%)	20 48
9	J	424/548 (77%)	382 (90%)	42 (10%)	8 29
9	K	423/548 (77%)	379 (90%)	44 (10%)	7 28
10	L	155/169 (92%)	136 (88%)	19 (12%)	4 23
11	M	55/67 (82%)	42 (76%)	13 (24%)	1 4
12	N	460/724 (64%)	398 (86%)	62 (14%)	4 21
13	O	576/650 (89%)	478 (83%)	98 (17%)	2 13
14	R	304/411 (74%)	290 (95%)	14 (5%)	27 54
15	S	8/195 (4%)	8 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	X	406/513 (79%)	373 (92%)	33 (8%)	11 39
16	Y	416/513 (81%)	375 (90%)	41 (10%)	8 29
All	All	6889/9715 (71%)	6050 (88%)	839 (12%)	8 23

5 of 839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	K	128	ILE
12	N	544	LEU
16	Y	49	LEU
9	K	231	LEU
9	K	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	556	GLN
16	Y	505	ASN
13	O	753	ASN
16	X	95	ASN
6	H	494	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	6
14	R	2
16	X	1
1	A	1
6	H	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	510:GLY	C	511:SER	N	3.32
1	N	213:TYR	C	214:ARG	N	3.24
1	X	386:MET	C	387:GLY	N	3.24
1	N	92:TRP	C	93:ASN	N	3.21
1	R	388[A]:CYS	C	389:SER	N	3.09

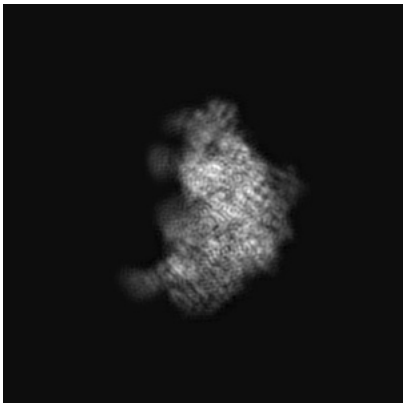
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3385. These allow visual inspection of the internal detail of the map and identification of artifacts.

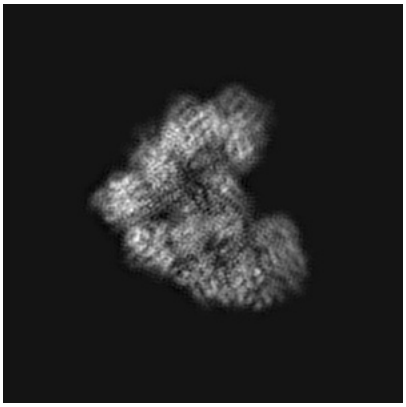
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

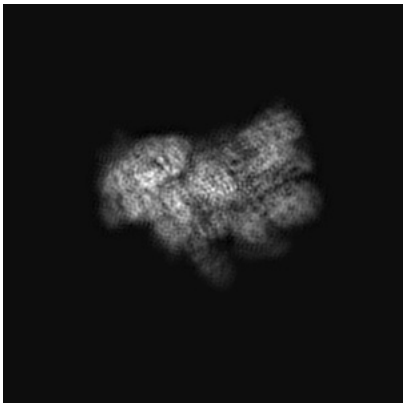
6.1.1 Primary map



X



Y

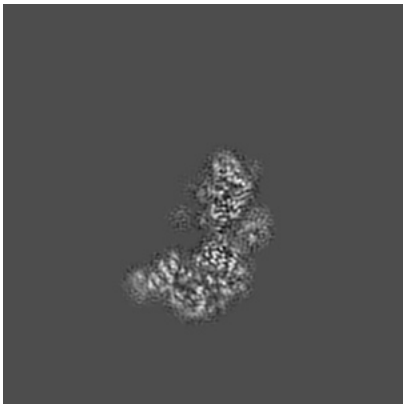


Z

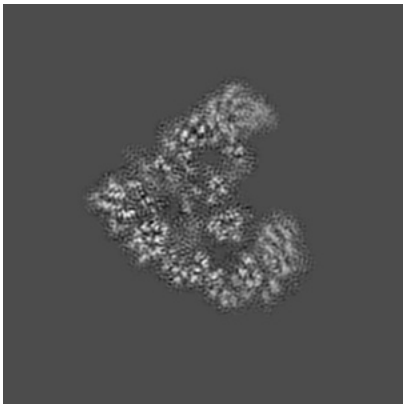
The images above show the map projected in three orthogonal directions.

6.2 Central slices

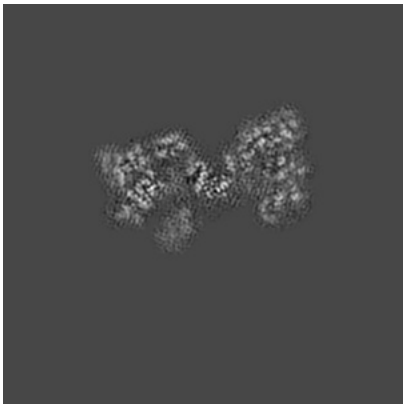
6.2.1 Primary map



X Index: 142



Y Index: 142



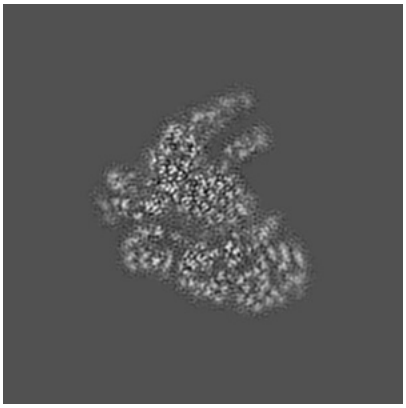
Z Index: 142

The images above show central slices of the map in three orthogonal directions.

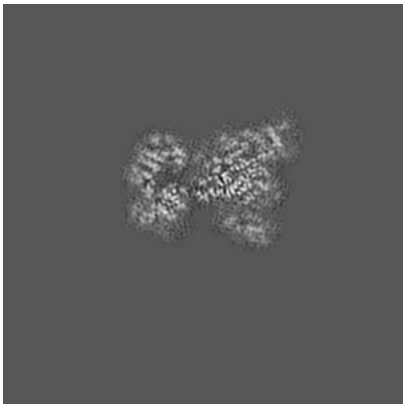
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 121



Y Index: 156

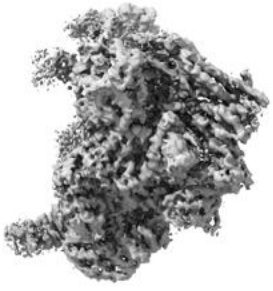


Z Index: 113

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

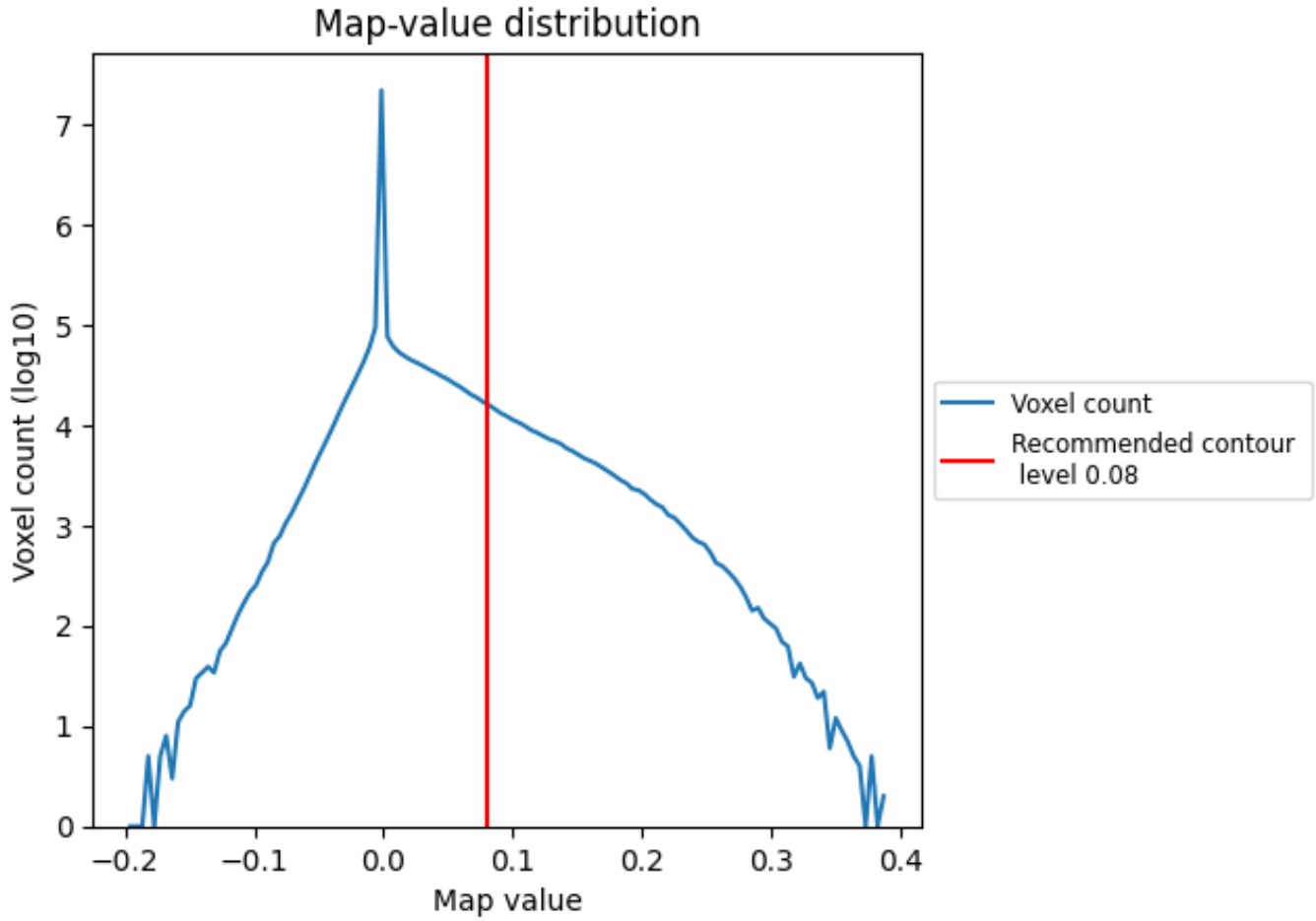
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

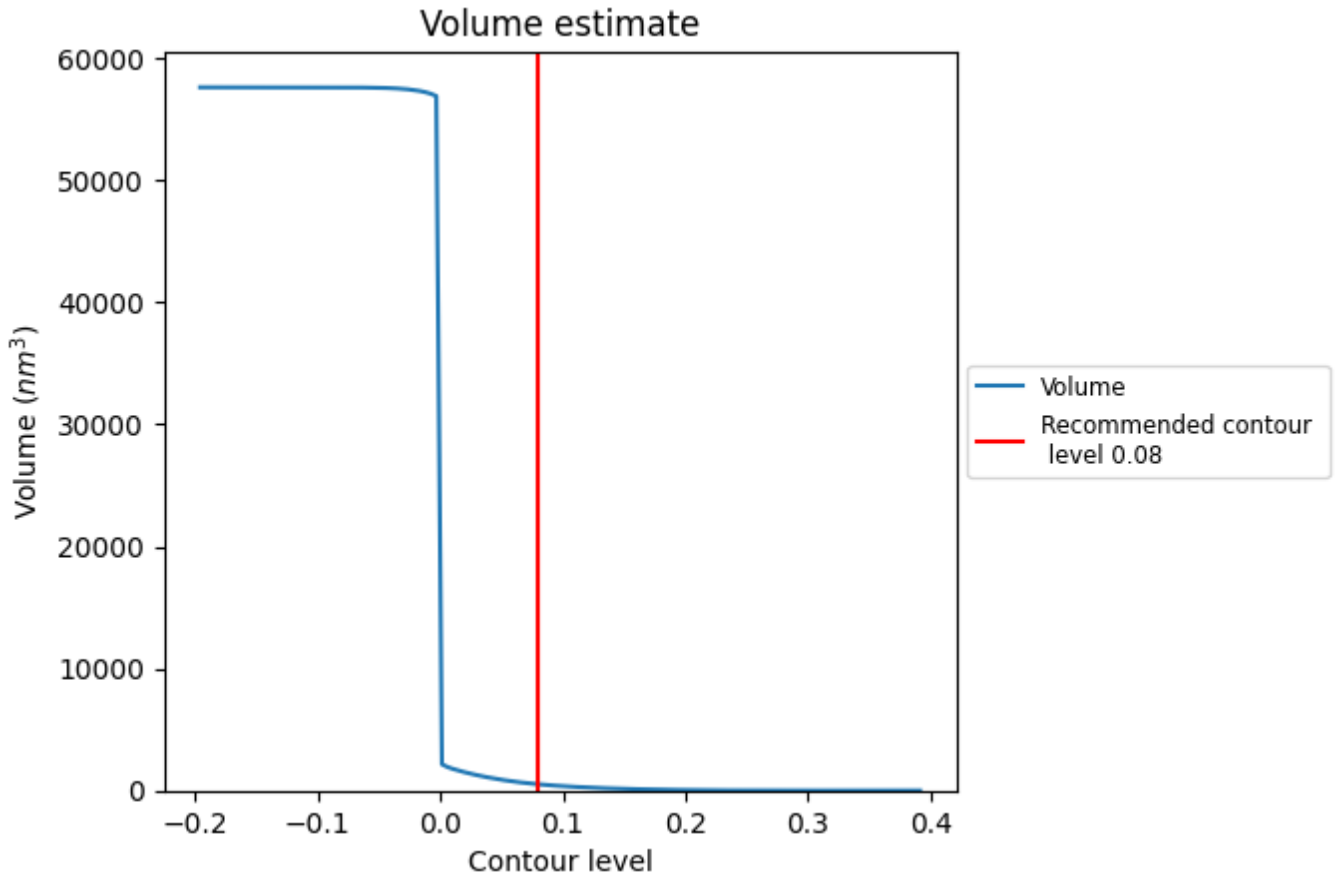
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

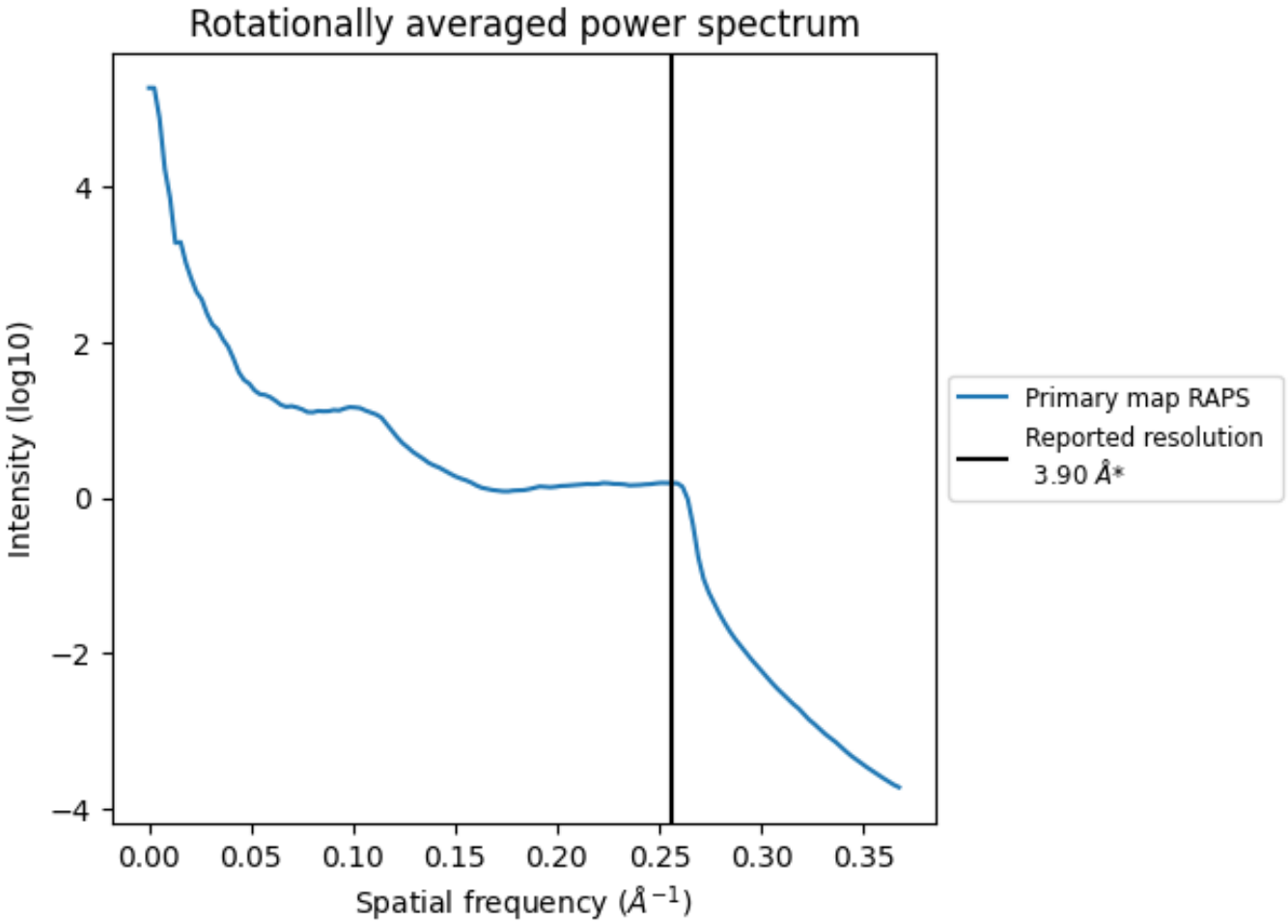
7.2 Volume estimate (i)



The volume at the recommended contour level is 516 nm^3; this corresponds to an approximate mass of 466 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

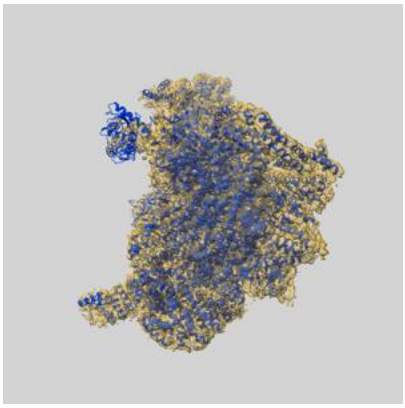
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

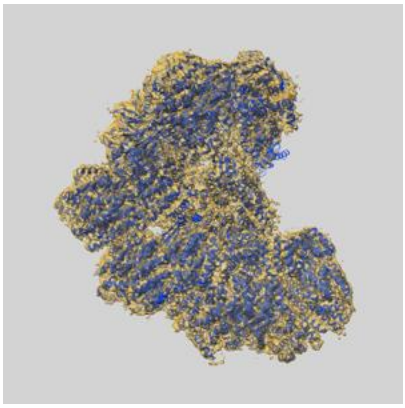
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3385 and PDB model 5G04. Per-residue inclusion information can be found in section 3 on page 7.

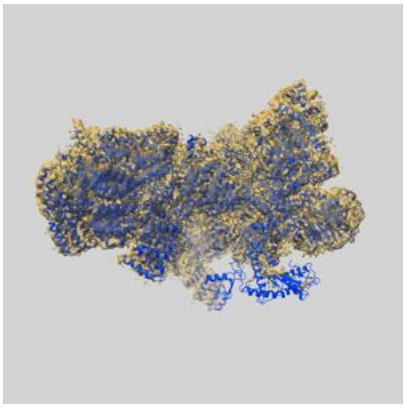
9.1 Map-model overlay



X



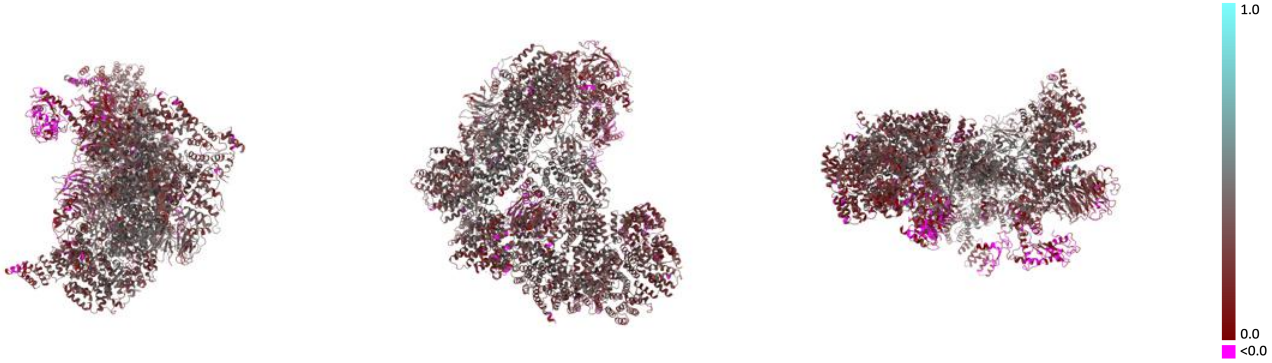
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

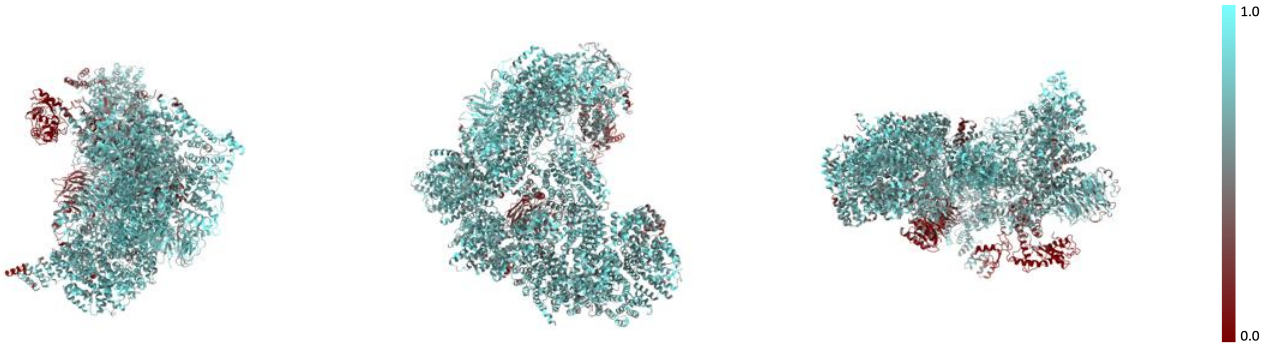
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

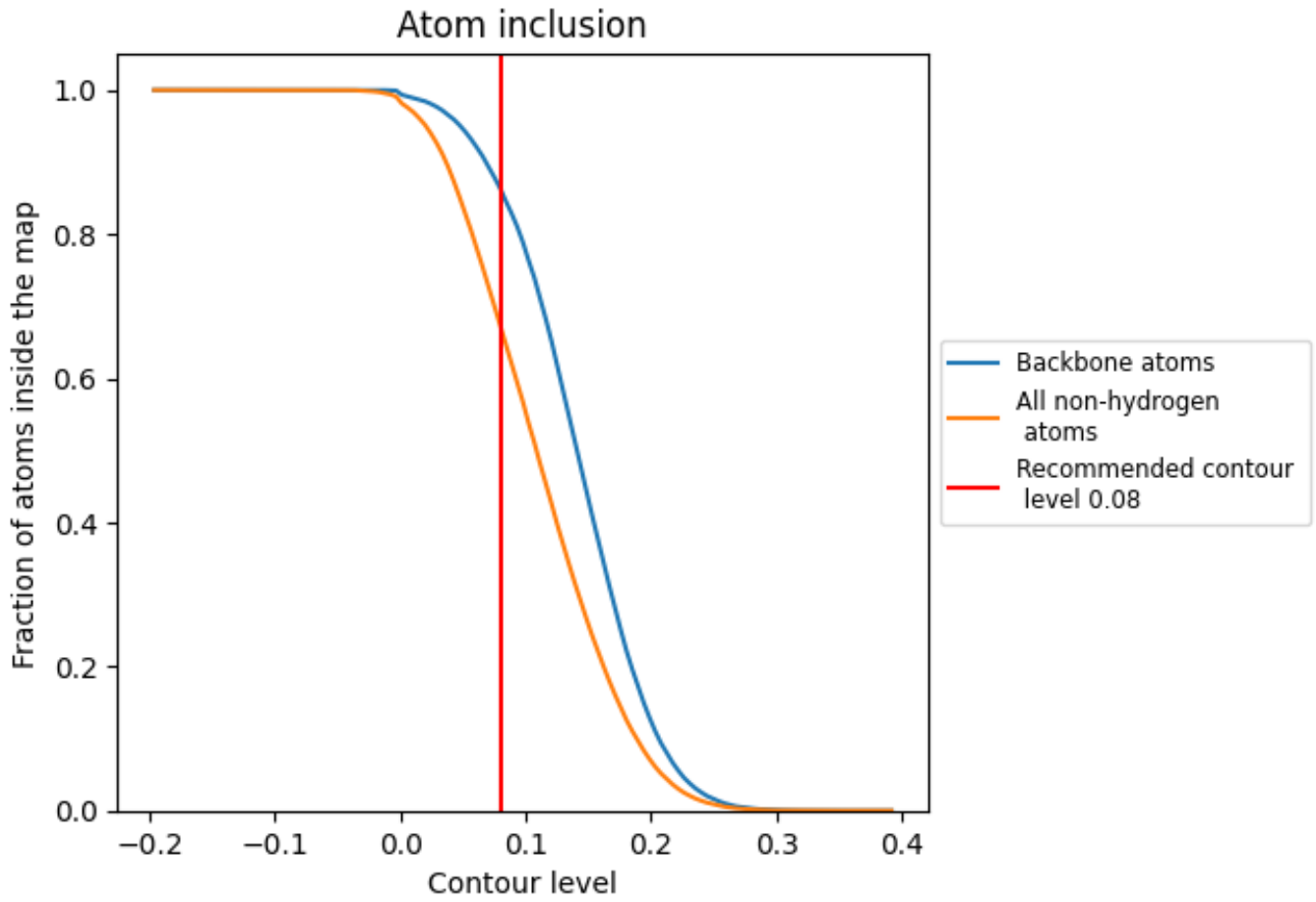
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6718	0.2990
A	0.7500	0.3600
B	0.0126	-0.0160
C	0.7182	0.3580
D	0.6991	0.3480
E	0.7050	0.3400
F	0.7375	0.3320
G	0.7512	0.3370
H	0.7567	0.3410
I	0.6692	0.2710
J	0.7630	0.3370
K	0.7337	0.3110
L	0.7026	0.3400
M	0.6294	0.3370
N	0.4352	0.1830
O	0.7416	0.3550
P	0.7135	0.3010
R	0.2669	0.1400
S	0.0857	0.0850
W	0.6341	0.3120
X	0.6322	0.2210
Y	0.6881	0.2530